

tert-Butyl alcohol
75-65-0 | DTXSID8020204

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 97.0 °C

Global applicability domain: Inside

Local applicability domain index: 8.62e-01

Confidence level: 7.92e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>tert-Butyl alcohol</div> <div>Measured: 82.4</div> <div>Predicted: 97.0</div>	<div>Image not found</div> <div>2-Butanol</div> <div>Measured: 99.5</div> <div>Predicted: 103</div>	<div>Image not found</div> <div>2-Methyl-1-propanol</div> <div>Measured: 108</div> <div>Predicted: 105</div>
<div>Image not found</div> <div>1-Butanol</div> <div>Measured: 118</div> <div>Predicted: 109</div>	<div>Image not found</div> <div>Butan-1-(2H)ol</div> <div>Measured: 118</div> <div>Predicted: 109</div>	<div>Image not found</div> <div>2-Methoxyethanol</div> <div>Measured: 124</div> <div>Predicted: 123</div>